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Abstract

We derive some estimates of the rate of convergence of Schwarz Waveform Relaxation (SWR) methods for the Schrödinger equation using an arbitrary number of subdomains. Hence, we justify that under certain conditions, the rates of convergence mathematically obtained for two subdomains [6, 7, 8] are still asymptotically valid for a larger number of subdomains, as it is usually numerically observed [22].

Keywords: Schrödinger equation; Schwarz Waveform Relaxation; domain decomposition method; asymptotic convergence rate

1. Introduction

We are interested in this paper in the analysis of the rate of convergence of some SWR methods by using an arbitrary number of subdomains. This study is an extension of existing results about the convergence of SWR algorithms on 2 subdomains [6, 7, 8]. We show that the convergence rates established for 2 subdomains are actually still accurate estimates for an arbitrary number of sufficiently large subdomains and bounded potentials. In this paper, we will mainly focus on the computation of contraction factors from Lipschitz continuous mappings involved in the proof of convergence of SWR methods. As a consequence, we will not introduce technical details about the full proof of convergence. Instead, we refer to several papers where the reader could find all the details of these proofs depending on the equation under consideration. For linear advection and diffusion reaction equations, we refer to [16]. The analysis and derivation for the Schrödinger equation in the time-dependent case is presented in [8, 9, 14, 15], while the stationary equation is studied in [6, 7].

The SWR algorithms are well-established methods for the parallel solution of evolution partial differential equations by allowing computations of the underlying PDE on small subdomains with very good speed-up. The convergence of the overall SWR methods is strongly

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dependent on the choice of the transmission conditions between the subdomain interfaces. Typically, Dirichlet transmission conditions will usually provide very slow convergence, while transparent transmissions boundary conditions provide a very fast convergence. In this paper, we do not discuss the space discretization of the algorithm but only focus on the convergence of the continuous in-space algorithms. We refer to [1, 15, 16, 17, 18, 19, 20, 21, 22, 23] for details about the SWR methods.

This paper is organized as follows. In section 2, we analyze the rate of convergence of the CSWR (Classical SWR) and OSWR (Optimized SWR) methods for the stationary Schrödinger equation solved by the imaginary-time method. The analysis is extended in Section 3, and some numerical experiments are proposed in Section 4.

2. Stationary states problems

We study the convergence of the SWR methods by using an arbitrary number $m \geqslant 2$ of subdomains, for computing the point spectrum of the Schrödinger Hamiltonian using the imaginary-time method [2, 3, 4, 5, 10, 11, 12, 13]. More specifically, we intend to determine the ground state to the following Schrödinger Hamitonian: $-\triangle + V(x)$, where the potential V is supposed to be smooth and bounded with bounded derivatives. The imaginary-time method reads, also called Normalized Gradient Flow method (NGF), for $t_0 = 0 < t_1 < \cdots < t_n < t_{n+1} < \cdots$

$$\begin{cases} \partial_t \phi(t,x) = \triangle\phi(t,x) - V(x)\phi(t,x)\phi(t,x),\, x \in \Omega,\, t_n < t < t_{n+1}, \\ \\ \phi(t,x) = 0,\, x \in \partial\Omega,\, t_n < t < t_{n+1}, \\ \\ \phi(t_{n+1},x) := \phi(,t_{n+1}^+,x) = \dfrac{\phi(t_{n+1}^-,x)}{||\phi(\cdot,t_{n+1}^-)||_{L^2(\mathbb{R})}}, \\ \\ \phi(0,x) = \varphi_0(x),\, x \in \mathbb{R}, \text{with } ||\varphi_0||^2_{L^2(\mathbb{R})} = 1, \end{cases} \tag{1}$$

where φ_0 is a given initial guess, usually built from an ansatz. The procedure is repeated until the convergence is reached, that is when the following stopping criterion is satisfied

$$||\phi(t_{n+1},\cdot) - \phi(t_n,\cdot)||_{L^\infty(\mathbb{R})} \leqslant \delta, \tag{2}$$

for $\delta > 0$ small enough. We propose the following decomposition (with possible overlap): $\Omega = \cup_{i=1}^m \Omega_i$, such that $\Omega_i = (\xi_i^-, \xi_i^+)$, for $2 \leqslant i \leqslant m-1$, $\Omega_1 = (-a, \xi_1^+)$ and $\Omega_m = (\xi_m^-, +a)$ (see Fig. 1). Moreover, the overlapping size is: $\xi_i^+ - \xi_{i+1}^- = \varepsilon > 0$, and $|\Omega_i| = L + \varepsilon$, where L is assumed to be much larger than ε. We also have $\xi_{i+1}^{\pm} - \xi_i^{\pm} = L$.

We study the convergence rate of the CSWR and OSWR algorithms. The convergence rate is defined as the slope of the logarithm residual history with respect to the Schwarz iteration number, i.e. $\{(k, \log(E^{(k)}))\,:\, k \in \mathbb{N}\}$, where

$$E^{(k)} := \sum_{i=1}^m \Big\| \; \|\phi^{\mathrm{cvg},(k)}_{i\big|(\xi_{i+1}^-,\xi_i^+)} - \phi^{\mathrm{cvg},(k)}_{i+1\big|(\xi_{i+1}^-,\xi_i^+)}\|_{\infty,\Gamma_\varepsilon} \Big\|_{L^2(0,T^{(k^{\mathrm{cvg}})})} \leqslant \delta^{\mathrm{Sc}}, \tag{3}$$

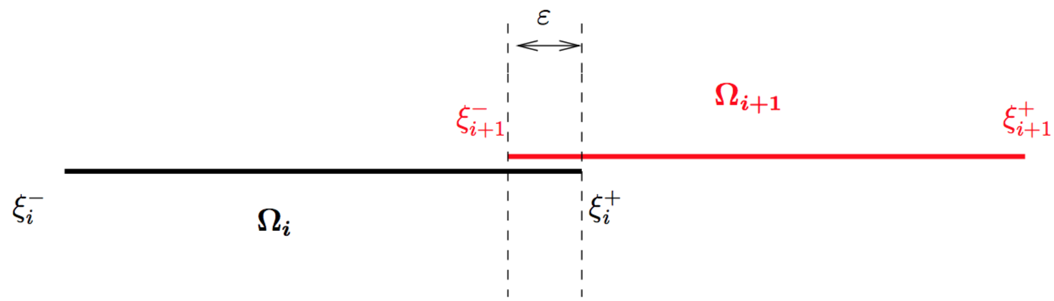

Figure 1: Domain decomposition with possible overlapping.

$\phi_i^{\mathrm{cvg},(k)}$ (resp. $T^{(k^{\mathrm{cvg}})}$) denotes the NGF converged solution (resp. time) in Ω_i at Schwarz iteration k, and δ^{Sc} is a small parameter. More specifically, we intend to prove that the convergence rate is independent of the number of subdomains as already numerically mentioned in [22] and Section 4. Finally, $\phi_i^{(k)}$ is the local solution in Ω_i for any $i \in \{1, \cdots, m\}$, at Schwarz iteration $k \in \mathbb{N}$.

2.1. Potential-free equation

We first consider the potential-free Schrödinger equation in imaginary-time, with $P(\partial_t, \partial_x) = \partial_t - \partial_x^2$. The NGF algorithm consists in solving for any $n \in \mathbb{N}$, from t_n to t_{n+1^-}:

$$\left\{\begin{array}{lcll} \left(\partial_t - \partial_x^2\right)\phi(t,x) & = & 0, & (t,x) \in (t_n, t_{n+1}^-) \times \Omega, \\ \phi(t,-a) & = & 0, & t \in (t_n, t_{n+1}^-), \\ \phi(t,a) & = & 0, & t \in (t_n, t_{n+1}^-). \end{array}\right.$$

Then, we normalize the solution $\phi(t_{n+1}, \cdot) = \phi(t_{n+1^-}, \cdot)/\|\phi(t_{n+1^-})\|_{L^2(\Omega)}$. The procedure is repeated until convergence following (2). Let us start by studying the rate of convergence of the CSWR, then considering the OSWR algorithm.

2.1.1. CSWR algorithm

The CSWR algorithm reads as follows: for $k \geqslant 1$ and $i \in \{2, \cdots, m-1\}$ from time t_n to t_{n+1^-}, solve

$$\left\{\begin{array}{lcll} P(\partial_t, \partial_x)\phi_i^{(k)} & = & 0, & (t,x) \in (t_n, t_{n+1}^-) \times \Omega_i, \\ \phi_i^{(k)}(0, \cdot) & = & \varphi_0, & x \in \Omega_i, \\ \phi_i^{(k)}(t, \xi_i^+) & = & \phi_{i+1}^{(k-1)}(t, \xi_i^+), & t \in (t_n, t_{n+1}^-), \\ \phi_i^{(k)}(t, \xi_i^-) & = & \phi_{i-1}^{(k-1)}(t, \xi_i^-), & t \in (t_n, t_{n+1}^-). \end{array}\right.$$

In Ω_1, we get

$$\left\{\begin{array}{lcl} P(\partial_t,\partial_x)\phi_1^{(k)} & = & 0, \qquad (t,x)\in(t_n,t_{n+1}^-)\times\Omega_1,\\ \phi_1^{(k)}(0,\cdot) & = & \varphi_0, \qquad x\in\Omega_1,\\ \phi_1^{(k)}(t,-a) & = & 0, \qquad t\in(t_n,t_{n+1}^-),\\ \phi_1^{(k)}(t,\xi_1^+) & = & \phi_2^{(k-1)}(t,\xi_2^+), \qquad t\in(t_n,t_{n+1}^-), \end{array}\right.$$

and in Ω_m

$$\left\{\begin{array}{lcl} P(\partial_t,\partial_x)\phi_m^{(k)} & = & 0, \qquad (t,x)\in(t_n,t_{n+1}^-)\times\Omega_m,\\ \phi_m^{(k)}(0,\cdot) & = & \varphi_0, \qquad x\in\Omega_m,\\ \phi_i^{(k)}(t,\xi_m^-) & = & \phi_{m-1}^{(k-1)}(t,\xi_m^-), \qquad t\in(t_n,t_{n+1}^-),\\ \phi_m^{(k)}(t,+a) & = & 0, \qquad t\in(t_n,t_{n+1}^-). \end{array}\right.$$

To analyze the convergence of this DDM, we set $e_i := \phi_{\text{exact}|\Omega_i} - \phi_i$ and we introduce $h_i^\pm \in H_0^{3/4}(0,T) = \big\{\phi \in H^{3/4}(0,T) \ : \ \phi(0) = 0\big\}$, for $i \in \{1,\cdots,m\}$. We then consider the following system, where we denote by τ the dual variable to t in Fourier space, and by $\widehat{\cdot}$ the Fourier transform with respect to t,

$$\left\{\begin{array}{lcl} \big(\mathtt{i}\tau - \partial_x^2\big)\widehat{e}_i(\tau,x) & = & 0, \qquad (\tau,x)\in\mathbb{R}\times\Omega_i,\\ \widehat{e}_i(\tau,\xi^\pm) & = & \widehat{h}_i^\pm(\tau), \qquad \tau\in\mathbb{R}\,. \end{array}\right.$$

We set $\alpha(\tau) := e^{\mathtt{i}\pi/4}\sqrt{\tau}$, and we get, for any $\tau\in\mathbb{R}$,

$$\widehat{e}_i(\tau,x) \;=\; A_i(\tau)e^{\alpha(\tau)x} + B_i(\tau)e^{-\alpha(\tau)x}$$

and for $i \in \{2,\cdots,m-1\}$

$$\widehat{e}_i(\tau,\xi_i^\pm) \;=\; A_i(\tau)e^{\alpha(\tau)\xi_i^\pm} + B_i(\tau)e^{\alpha(\tau)\xi_i^\pm} \;=\; h_i^\pm(\tau)\,.$$

By using the boundary conditions, we find, for $i \in \{2,\cdots,m-1\}$,

$$\left\{\begin{array}{lcl} A_i(\tau) & = & \dfrac{1}{e^{\alpha(\tau)(L+\varepsilon)} - e^{-\alpha(\tau)(L+\varepsilon)}}\Big(\widehat{h}_i^+(\tau)e^{-\alpha(\tau)\xi_i^-} - \widehat{h}_i^-(\tau)e^{-\alpha(\tau)\xi_i^+}\Big),\\ B_i(\tau) & = & \dfrac{1}{e^{\alpha(\tau)(L+\varepsilon)} - e^{-\alpha(\tau)(L+\varepsilon)}}\Big(\widehat{h}_i^-(\tau)e^{\alpha(\tau)\xi_i^-} - \widehat{h}_i^+(\tau)e^{\alpha(\tau)\xi_i^+}\Big)\,. \end{array}\right.$$

Similarly, we have

$$\left\{\begin{array}{lcl} A_1(\tau) & = & \dfrac{\widehat{h}_1^+(\tau)}{e^{\alpha(\tau)(L+\varepsilon/2-a)} - e^{-\alpha(\tau)(L+\varepsilon/2+a)}},\\ B_1(\tau) & = & \dfrac{\widehat{h}_1^+(\tau)}{e^{\alpha(\tau)(L+\varepsilon/2+a)} - e^{-\alpha(\tau)(L+\varepsilon/2-a)}}, \end{array}\right.$$

and

$$\left\{\begin{array}{lcl} A_m(\tau) &=& \dfrac{\widehat{h}_m^-(\tau)}{e^{\alpha(\tau)(a-L-\varepsilon/2)}-e^{\alpha(\tau)(L+\varepsilon/2+a)}}, \\ B_m(\tau) &=& -\dfrac{\widehat{h}_m^-(\tau)}{e^{-\alpha(\tau)(L+\varepsilon/2+a)}-e^{\alpha(\tau)(L+\varepsilon/2-a)}}. \end{array}\right.$$

We introduce a mapping $\mathcal{G}^{(C)}$ from $\left(H^{3/4}(\mathbb{R})\right)^{2m}$ to itself, defined as follows

$$\mathcal{G}^{(C)}:\langle\left\{h_i^+(t),h_{i+1}^-(t)\right\}_{1\leqslant i\leqslant m}\rangle=\langle\left\{e_i(t,\xi_{i+1}^-),e_{i+1}(t,\xi_i^+)\right\}_{1\leqslant i\leqslant m}\rangle.$$

Thus, we deduce that

$$\widehat{\mathcal{G}}^{(C)}:\langle\left\{\widehat{h}_i^+(\tau),\widehat{h}_{i+1}^-(\tau)\right\}_{1\leqslant i\leqslant m}\rangle=\langle\left\{\widehat{e}_i(\tau,\xi_{i+1}^-),\widehat{e}_{i+1}(\tau,\xi_i^+)\right\}_{1\leqslant i\leqslant m}\rangle,$$

where, for $i\in\{2,\cdots,m-1\}$,

$$\widehat{e}_i(\tau,\xi_{i+1}^-)=\frac{1}{e^{\alpha(\tau)(L+\varepsilon)}-e^{-\alpha(\tau)(L+\varepsilon)}}\Big(\widehat{h}_i^-(\tau)(e^{\varepsilon\alpha(\tau)}-e^{-\varepsilon\alpha(\tau)})+\widehat{h}_i^+(\tau)(e^{L\alpha(\tau)}-e^{-L\alpha(\tau)})\Big)$$

and

$$\widehat{e}_{i+1}(\tau,\xi_i^+)=\frac{1}{e^{\alpha(\tau)(L+\varepsilon)}-e^{-\alpha(\tau)(L+\varepsilon)}}\Big(\widehat{h}_{i+1}^+(\tau)(e^{\varepsilon\alpha(\tau)}-e^{-\varepsilon\alpha(\tau)})+\widehat{h}_{i+1}^-(\tau)(e^{L\alpha(\tau)}-e^{-L\alpha(\tau)})\Big).$$

Following the same strategy as for the two subdomains case, see [7, 22], we compute $\widehat{\mathcal{G}}^{(C),2}\big(\langle\{\widehat{h}_i^+,\widehat{h}_{i+1}^-\}_i\rangle\big)$. Let us set $\widehat{h}_i^{+,(2)}(\tau):=\widehat{e}_i(\tau,\xi_{i+1}^-)$ and $\widehat{h}_{i+1}^{-,(2)}(\tau):=\widehat{e}_{i+1}(\tau,\xi_i^+)$, we get for $i\in\{2,\cdots,m-1\}$

$$\widehat{e}_i^{(2)}(\tau,\xi_{i+1}^-)=\frac{1}{e^{\alpha(\tau)(L+\varepsilon)}-e^{-\alpha(\tau)(L+\varepsilon)}}\Big(\widehat{e}_i(\tau,\xi_{i+1}^-)\big(e^{\alpha(\tau)L}-e^{-\alpha(\tau)L}\big)+\widehat{e}_i(\tau,\xi_{i-1}^+)\big(e^{\alpha(\tau)\varepsilon}-e^{-\alpha(\tau)\varepsilon}\big)\Big)$$

and

$$\widehat{e}_{i+1}^{(2)}(\tau,\xi_i^+)=\frac{1}{e^{\alpha(\tau)(L+\varepsilon)}-e^{-\alpha(\tau)(L+\varepsilon)}}\Big(\widehat{e}_{i+1}(\tau,\xi_i^+)\big(e^{\alpha(\tau)L}-e^{-\alpha(\tau)L}\big)+\widehat{e}_{i+1}(\tau,\xi_{i+2}^-)\big(e^{\alpha(\tau)\varepsilon}-e^{-\alpha(\tau)\varepsilon}\big)\Big).$$

We then obtain

$$\begin{array}{rcl}\widehat{e}_{i+1}^{(2)}(\tau,\xi_i^+) &=& \dfrac{1}{\big(e^{\alpha(\tau)(L+\varepsilon)}-e^{-\alpha(\tau)(L+\varepsilon)}\big)^2}\Big\{\widehat{h}_{i+1}^-(\tau)\big(e^{\alpha(\tau)L}-e^{-\alpha(\tau)L}\big)^2+\widehat{h}_{i+1}^-(\tau)\big(e^{\alpha(\tau)\varepsilon}-e^{-\alpha(\tau)\varepsilon}\big)^2 \\ && +\widehat{h}_{i+1}^-(\tau)\big(e^{\alpha(\tau)L}-e^{-\alpha(\tau)L}\big)^2+2\widehat{h}_{i+1}^+(\tau)\big(e^{\alpha(\tau)\varepsilon}-e^{-\alpha(\tau)\varepsilon}\big)\big(e^{\alpha(\tau)L}-e^{-\alpha(\tau)L}\big)\Big\} \\ &=& \dfrac{e^{-2\varepsilon\alpha(\tau)}}{1-e^{-2\alpha(\tau)(L+\varepsilon)}\big)^2}\Big\{\widehat{h}_{i+1}^-(\tau)\big(1-e^{-2\alpha(\tau)L}\big)^2+\widehat{h}_{i+1}^-(\tau)\big(e^{\alpha(\tau)(\varepsilon-2L)}-e^{-\alpha(\tau)(\varepsilon-2L)}\big)^2 \\ && +2\widehat{h}_{i+1}^+(\tau)\big(e^{\alpha(\tau)\varepsilon}-e^{-\alpha(\tau)\varepsilon}\big)\big(e^{-\alpha(\tau)L}-e^{-3\alpha(\tau)L}\big)\Big\}\end{array}$$

and

$$\begin{aligned}\widehat{e}_i^{(2)}(\tau,\xi_{i+1}^-) &= \frac{1}{\big(e^{\alpha(\tau)(L+\varepsilon)}-e^{-\alpha(\tau)(L+\varepsilon)}\big)^2}\Big\{\widehat{h}_i^+(\tau)\big(e^{\alpha(\tau)L}-e^{-\alpha(\tau)L}\big)^2+\widehat{h}_i^+(\tau)\big(e^{\alpha(\tau)\varepsilon}-e^{-\alpha(\tau)\varepsilon}\big)^2\\ &\quad +2\widehat{h}_i^-(\tau)\big(e^{\alpha(\tau)\varepsilon}-e^{-\alpha(\tau)\varepsilon}\big)\big(e^{\alpha(\tau)L}-e^{-\alpha(\tau)L}\big)\Big\}\\ &= \frac{e^{-2\alpha(\tau)\varepsilon}}{\big(1-e^{-2\alpha(\tau)(L+\varepsilon)}\big)^2}\Big\{\widehat{h}_i^+(\tau)\big(1-e^{-2\alpha(\tau)L}\big)^2+\widehat{h}_i^+(\tau)\big(e^{\alpha(\tau)(\varepsilon-2L)}-e^{-\alpha(\tau)(\varepsilon-2L)}\big)^2\\ &\quad +2\widehat{h}_i^-(\tau)\big(e^{\alpha(\tau)\varepsilon}-e^{-\alpha(\tau)\varepsilon}\big)\big(e^{-\alpha(\tau)L}-e^{-3\alpha(\tau)L}\big)\Big\}.\end{aligned}$$

For $m \geqslant 2$ subdomains, we have

$$\widehat{\mathcal{G}}^{(C),2}\big(\langle\{\widehat{h}_i^+(\tau),\widehat{h}_{i+1}^-(\tau)\}_i\rangle\big) = e^{-2\alpha(\tau)\varepsilon}\langle\big\{\widehat{h}_i^+(\tau),\widehat{h}_{i+1}^-(\tau)\big\}_i\rangle+O\big(e^{-\alpha(\tau)L}\big).$$

In particular, for $\tau<0$, we obtain

$$\big|\widehat{\mathcal{G}}^{(C),2}\big(\langle\{\widehat{h}_i^+(\tau),\widehat{h}_{i+1}^-(\tau)\}_i\rangle\big)\big| \leqslant e^{-\varepsilon\sqrt{2|\tau|}}\big|\langle\big\{\widehat{h}_i^+(\tau),\widehat{h}_{i+1}^-(\tau)\big\}_i\rangle\big|+Ce^{-L\sqrt{2|\tau|}}.$$

We then get

$$\big\|\mathcal{G}^{(C),2}\big(\langle\{\widehat{h}_i^+,\widehat{h}_{i+1}^-\}_i\rangle\big)\big\|_{\left(H^{3/4}(t_n,t_{n+1}^-)\right)^{2m}} \leqslant C\big\|\big(\langle\{\widehat{h}_i^+,\widehat{h}_{i+1}^-\}_i\rangle\big)\big\|,$$

with C a positive constant lower that 1. We also have

$$\frac{d^2\widehat{e}_i}{dx^2}(\tau,x) = \alpha^2(\tau)\widehat{e}_i(\tau,x).$$

Then, one gets

$$\begin{aligned}\|e_i\|_{L^2(0,T;H^2(\Omega_i))} &\leqslant \int_{\mathbb{R}}\int_{\Omega_i}\frac{|\alpha(\tau)|^4}{|\alpha(\tau)||e^{\alpha(\tau)(L+\varepsilon)}-e^{-\alpha(\tau)(L+\varepsilon)}|}\big(|\widehat{h}_i^+(\tau)|(|e^{-\alpha(\tau)(\xi_i^- x)}|+|e^{-\alpha(\tau)(x-\xi_i^+)}|)+\\ &\quad |\widehat{h}_i^-(\tau)|(|e^{-\alpha(\tau)(\xi_i^+-x)}|+|e^{-\alpha(\tau)(x-\xi_i^-)}|)\big)dx\end{aligned}$$

Je ne sais pas trop ce que tu veux ecrire

$$\|\|\|_{\Pi_{i=1}^m H^{2,1}(\Omega_i\times(0,T))} \leqslant$$

This justifies the fact that, as numerically observed in [22] and in Section 4, the convergence rate is independent of the number of subdomains of length L. However, the overall convergence is linearly dependent of the number of subdomains through the summation over the m subdomains in (3). As a consequence, we expect that the logscale slope of the residual history, i.e. the convergence rate, to be independent of m. Finally, the overall error $\{(k,E^{(k)})\}$ is still shifted in logscale, by a positive constant linearly dependent on $\log(m)$.

We conclude by the following

Proposition 2.1. *The convergence rate $C_\varepsilon^{(C)}$ of the CSWR method with subdomains of length L is of the form*

$$C_\varepsilon^{(C)} = \sup_{\tau\in\mathbb{R}} e^{-\varepsilon\sqrt{2|\tau|}}+O\big(e^{-L\sqrt{2|\tau|}}\big).$$

2.2. OSWR algorithm

We now study the OSWR algorithm for $m \geqslant 2$ subdomains. To this end, we define the transparent boundary operator $\partial_x \pm \partial_t^{1/2}$. The OSWR algorithm reads as follows: for $k \geqslant 1$ and for $i \in \{2, \cdots, m-1\}$, solve

$$\left\{\begin{array}{lcl} P(\partial_t, \partial_x)\phi_i^{(k)} & = & 0, \qquad (t,x) \in (t_n, t_{n+1}^-) \times \Omega_i, \\ \phi_i^{(k)}(0,\cdot) & = & \varphi_0, \qquad x \in \Omega_i, \\ (\partial_x + \partial_t^{1/2})\phi_i^{(k)}(t,\xi_i^+) & = & (\partial_x + \partial_t^{1/2})\phi_{i+1}^{(k-1)}(t,\xi_i^+), \qquad t \in (t_n, t_{n+1}^-), \\ (\partial_x - \partial_t^{1/2})\phi_i^{(k)}(t,\xi_i^-) & = & (\partial_x - \partial_t^{1/2})\phi_{i-1}^{(k-1)}(t,\xi_i^-), \qquad t \in (t_n, t_{n+1}^-). \end{array}\right.$$

In Ω_1, we get

$$\left\{\begin{array}{lcl} P(\partial_t, \partial_x)\phi_1^{(k)} & = & 0, \qquad (t,x) \in (t_n, t_{n+1}^-) \times \Omega_1, \\ \phi_1^{(k)}(0,\cdot) & = & \varphi_0, \qquad x \in \Omega_1, \\ \phi_1^{(k)}(t,-a) & = & 0, \qquad t \in (t_n, t_{n+1}^-), \\ (\partial_x + \partial_t^{1/2})\phi_1^{(k)}(t,\xi_1^+) & = & (\partial_x + \partial_t^{1/2})\phi_2^{(k-1)}(t,\xi_1^+), \qquad t \in (t_n, t_{n+1}^-), \end{array}\right.$$

and in Ω_m

$$\left\{\begin{array}{lcl} P(\partial_t, \partial_x)\phi_m^{(k)} & = & 0, \qquad (t,x) \in (t_n, t_{n+1}^-) \times \Omega_m, \\ \phi_m^{(k)}(0,\cdot) & = & \varphi_0, \qquad x \in \Omega_m, \\ (\partial_x - \partial_t^{1/2})\phi_i^{(k)}(t,\xi_m^-) & = & (\partial_x - \partial_t^{1/2})\phi_{m-1}^{(k-1)}(t,\xi_m^-), \qquad t \in (t_n, t_{n+1}^-), \\ \phi_m^{(k)}(t,+a) & = & 0, \qquad t \in (t_n, t_{n+1}^-). \end{array}\right.$$

We then consider

$$\left\{\begin{array}{lcl} \big(\mathtt{i}\tau - \partial_x^2\big)\widehat{e}_i(\tau,x) & = & 0, \qquad (\tau,x) \in \mathbb{R} \times \Omega_i, \\ (\partial_x \pm \alpha(\tau))\widehat{e}_i(\tau,\xi^{\pm}) & = & \widehat{h}_i^{\pm}(\tau), \qquad \tau \in \mathbb{R}\,. \end{array}\right.$$

By defining $\alpha(\tau) := e^{\mathtt{i}\pi/4}\sqrt{\tau}$, we obtain

$$\widehat{e}_i(\tau,x) \;=\; A_i(\tau)e^{\alpha(\tau)x} + B_i(\tau)e^{-\alpha(\tau)x}\,.$$

By again using the boundary conditions, we find for $i \in \{2, \cdots, m-1\}$

$$A_i(\tau) = \frac{\widehat{h}_i^+(\tau)e^{-\alpha(\tau)\xi_i^+}}{2\alpha(\tau)}, \qquad B_i(\tau) = -\frac{\widehat{h}_i^-(\tau)e^{\alpha(\tau)\xi_i^-}}{2\alpha(\tau)}.$$

We introduce a mapping $\mathcal{G}^{(O)}$ defined as follows

$$\mathcal{G}^{(O)} : \langle \big\{h_i^+(t), h_{i+1}^-(t)\big\}_{1\leqslant i\leqslant m}\rangle = \langle \big\{(\partial_x + \partial_t^{1/2})e_{i+1}(t,\xi_i^+), (\partial_x - \partial_t^{1/2})e_i(t,\xi_{i+1}^-)\big\}_{1\leqslant i\leqslant m}\rangle\,.$$

Thus, we can write that

$$\begin{array}{rcl} \widehat{\mathcal{G}}^{(O)} : \langle \big\{\widehat{h}_i^+(\tau), \widehat{h}_{i+1}(\tau)\big\}_{1\leqslant i\leqslant m}\rangle & = & \langle \big\{(\partial_x + \alpha(\tau))\widehat{e}_{i+1}(\tau,\xi_i^+), (\partial_x - \alpha(\tau))\widehat{e}_i(\tau,\xi_{i+1}^-)\big\}_{1\leqslant i\leqslant m}\rangle \\ & = & 2\alpha(\tau)\langle \big\{A_{i+1}(\tau)e^{\alpha(\tau)\xi_i^+}, -B_i(\tau)e^{-\alpha(\tau)\xi_{i+1}^-}\big\}_{1\leqslant i\leqslant m}\rangle. \end{array}$$

where for $i \in \{2, \cdots, m-1\}$. Let us introduce

$$\widehat{h}_i^{+,(2)}(\tau) = 2\alpha(\tau) A_{i+1}(\tau) e^{\alpha(\tau)\xi_i^+}, \quad \widehat{h}_{i+1}^{-,(2)}(\tau) = -2\alpha(\tau) B_i(\tau) e^{-\alpha(\tau)\xi_{i+1}^-},$$

so that one gets: $\widehat{e}_i^{(2)}(\tau, x) = A_i^{(2)}(\tau) e^{\alpha(\tau)x} + B_i^{(2)}(\tau) e^{-\alpha(\tau)x}$. From the boundary conditions, we find, for $i \in \{2, \cdots, m-1\}$,

$$\begin{cases} A_i^{(2)}(\tau) & = & \dfrac{\widehat{h}_i^{+,(2)}(\tau) e^{-\alpha(\tau)\xi_i^+}}{2\alpha(\tau)} & = & A_{i+1}(\tau)\,, \\ B_i^{(2)}(\tau) & = & -\dfrac{\widehat{h}_i^{-,(2)}(\tau) e^{\alpha(\tau)\xi_i^-}}{2\alpha(\tau)} & = & B_{i-1}(\tau)\,. \end{cases}$$

In addition, we have

$$\begin{array}{rcl} \widehat{\mathcal{G}}^{(O),2} : \langle \{ \widehat{h}_i^+(\tau), \widehat{h}_{i+1}^-(\tau) \}_{1 \leqslant i \leqslant m} \rangle & = & \langle \{ (\partial_x + \alpha(\tau)) \widehat{e}_{i+1}^{(2)}(\tau, \xi_i^+), (\partial_x - \alpha(\tau)) \widehat{e}_i^{(2)}(\tau, \xi_{i+1}^-) \}_{1 \leqslant i \leqslant m} \rangle \\ & = & 2\alpha(\tau) \langle \{ A_{i+1}^{(2)}(\tau) e^{\alpha(\tau)\xi_i^+}, -B_i^{(2)}(\tau) e^{-\alpha(\tau)\xi_{i+1}^-} \}_{1 \leqslant i \leqslant m} \rangle \\ & = & \langle \{ \widehat{h}_{i+2}^+(\tau) e^{-\alpha(\tau)(\xi_{i+2}^+ - \xi_i^+)}, \widehat{h}_{i-1}^-(\tau) e^{-\alpha(\tau)(\xi_{i+1}^- - \xi_{i-1}^-)} \}_{1 \leqslant i \leqslant m} \rangle \\ & = & \langle \{ \widehat{h}_{i+2}^+(\tau) e^{-2\alpha(\tau)(L+\varepsilon)}, \widehat{h}_{i-1}^-(\tau) e^{-2\alpha(\tau)(L+\varepsilon)} \}_{1 \leqslant i \leqslant m} \rangle \end{array}$$

We can finally state the following result.

Proposition 2.2. *The convergence rate $C_\varepsilon^{(O)}$ of the OSWR method with subdomains of length L is $O\big(e^{-2\alpha(\tau)(L+\varepsilon)}\big)$.*

Remark 2.1. *Using a simple unitary transformation, it is trivial to extend the above results to the case of a linear equation with time-dependent potential $V(t)$ in $L^1_{loc}(\mathbb{R})$. Indeed, from*

$$\big(\mathtt{i}\partial_t + \partial_x^2 + V(t)\big)\phi(t, x) = 0,$$

it is sufficient to define the new unknown $\widetilde{\phi}(t, x) = e^{-\int_0^t V(s)} \phi(t, x)$ by gauge change, $\widetilde{\phi}$ satisfying then the potential-free Schrödinger equation.

2.3. The space variable potential case

We now assume that the potential is space-dependent. Then, the argument used in Remark 2.1 is longer valid. As it was studied in [7], we can no more get a simple expression of the exact solution on each subdomain, and we then have to use approximations. Let us set : $P(t, x, D) = \partial_t - \partial_x^2 - V(x)$, where V is smooth, bounded with bounded derivative.

2.3.1. CSWR algorithm

Using the same notations as above, we directly consider the error equation for the CSWR algorithm:

$$\begin{cases} \big(\mathtt{i}\tau - \partial_x^2 + V(x)\big)\widehat{e}_i(\tau, x) & = & 0, & (\tau, x) \in \mathbb{R} \times \Omega_i \\ \widehat{e}_i(\tau, \xi^\pm) & = & \widehat{h}_i^\pm(\tau), & \tau \in \mathbb{R} \end{cases} \tag{4}$$

We also assume that V is positive, and that $\|V\|_\infty$ exists. From Nirenberg's factorization theorem [7, 24]

$$P(t,x,\partial_t,\partial_x) = (\partial_x + i\Lambda^-)(\partial_x + i\Lambda^+) + \mathcal{R}, \tag{5}$$

where $\mathcal{R} \in \mathrm{OPS}^{-\infty}$ is a smoothing pseudodifferential operator. The operators $\Lambda^\pm$ are pseudodifferential operators of order 1/2 (in time) and order zero in x. Furthermore, their total symbols $\lambda^\pm := \sigma(\Lambda^\pm)$ can be expanded in $S_S^{1/2}$ as

$$\lambda^\pm \sim \sum_{j=0}^{+\infty} \lambda^\pm_{1/2-j/2}, \tag{6}$$

where $\lambda^\pm_{1/2-j/2}$ are symbols corresponding to operators of order $1/2 - j/2$, see [7]. We denote by $\mathfrak{e}_i$ an *approximate* solution to (4) in Ω_i of the following form (neglecting the scattering effects)

$$\widehat{\mathfrak{e}}_i(\tau,x) \;=\; \mathfrak{A}_i(\tau)\exp\big(-\mathtt{i}\int_{\xi_i^+}^x \lambda^+(y,\tau)dy\big) + \mathfrak{B}_i(\tau)\exp\big(-\mathtt{i}\int_{\xi_i^-}^x \lambda^-(y,\tau)dy\big).$$

By construction, $\lambda^- = -\lambda^+$ if we select $\lambda^+_{1/2} = -\lambda^-_{1/2}$ (see [7]). Now, by using the boundary conditions, we find that, for $i \in \{2,\cdots,m-1\}$,

$$\begin{cases} \mathfrak{A}_i(\tau) \;=\; \dfrac{\widehat{h}_i^+(\tau) - \widehat{h}_i^-(\tau)\exp\big(-\mathtt{i}\int_{\xi_i^-}^{\xi_i^+}\lambda^-(y,\tau)dy\big)}{1-\exp\big(-2\mathtt{i}\int_{\xi_i^-}^{\xi_i^+}\lambda^-(y,\tau)dy\big)}, \\[2ex] \mathfrak{B}_i(\tau) \;=\; \dfrac{\widehat{h}_i^-(\tau) - \widehat{h}_i^+(\tau)\exp\big(-\mathtt{i}\int_{\xi_i^-}^{\xi_i^+}\lambda^-(y,\tau)dy\big)}{1-\exp\big(-2\mathtt{i}\int_{\xi_i^-}^{\xi_i^+}\lambda^-(y,\tau)dy\big)}. \end{cases}$$

Let us introduce

$$\mathcal{G}^{(C)} : \langle \big\{h_i^+(t), h_{i+1}(t)\big\}_{1\leqslant i\leqslant m}\rangle = \langle \big\{\mathfrak{e}_i(t,\xi_{i+1}^-), \mathfrak{e}_{i+1}(t,\xi_i^+)\big\}_{1\leqslant i\leqslant m}\rangle\,,$$

thus we have

$$\widehat{\mathcal{G}}^{(C)} : \langle \big\{\widehat{h}_i^+(\tau), \widehat{h}_{i+1}(\tau)\big\}_{1\leqslant i\leqslant m}\rangle = \langle \big\{\widehat{\mathfrak{e}}_i(\tau,\xi_{i+1}^-), \widehat{\mathfrak{e}}_{i+1}(\tau,\xi_i^+)\big\}_{1\leqslant i\leqslant m}\rangle\,.$$

Next, some computations yield

$$\begin{aligned} \widehat{\mathfrak{e}}_i(\tau,x) \;=\; & \frac{\big(\widehat{h}_i^+(\tau) - \widehat{h}_i^-(\tau)\exp\big(-\mathtt{i}\int_{\xi_i^-}^{\xi_i^+}\lambda^-(y,\tau)dy\big)\big)\exp\big(\mathtt{i}\int_{\xi_i^+}^x \lambda^-(y,\tau)dy\big)}{1-\exp\big(-2\mathtt{i}\int_{\xi_i^-}^{\xi_i^+}\lambda^-(y,\tau)dy\big)} \\ & + \frac{\big(\widehat{h}_i^-(\tau) - \widehat{h}_i^+(\tau)\exp\big(-\mathtt{i}\int_{\xi_i^-}^{\xi_i^+}\lambda^-(y,\tau)dy\big)\big)\exp\big(-\mathtt{i}\int_{\xi_i^-}^x \lambda^-(y,\tau)dy\big)}{1-\exp\big(-2\mathtt{i}\int_{\xi_i^-}^{\xi_i^+}\lambda^-(y,\tau)dy\big)} \end{aligned}$$

and

$$\begin{aligned}
\widehat{\mathfrak{e}}_{i+1}(\tau,\xi_i^+) &= \frac{\big(\widehat{h}_{i+1}^+(\tau)-\widehat{h}_{i+1}^-(\tau)\exp\big(-\mathtt{i}\int_{\xi_{i+1}^-}^{\xi_{i+1}^+}\lambda^-(y,\tau)dy\big)\big)\exp\big(-\mathtt{i}\int_{\xi_i^+}^{\xi_{i+1}^+}\lambda^-(y,\tau)dy\big)}{1-\exp\big(-2\mathtt{i}\int_{\xi_{i+1}^-}^{\xi_{i+1}^+}\lambda^-(y,\tau)dy\big)} \\
&+\frac{\big(\widehat{h}_{i+1}^-(\tau)-\widehat{h}_{i+1}^+(\tau)\exp\big(-\mathtt{i}\int_{\xi_{i+1}^-}^{\xi_{i+1}^+}\lambda^-(y,\tau)dy\big)\big)\exp\big(-\mathtt{i}\int_{\xi_{i+1}^-}^{\xi_i^+}\lambda^-(y,\tau)dy\big)}{1-\exp\big(-2\mathtt{i}\int_{\xi_{i+1}^-}^{\xi_{i+1}^+}\lambda^-(y,\tau)dy\big)} \\
&= \frac{\big(\widehat{h}_{i+1}^+(\tau)-\widehat{h}_{i+1}^-(\tau)\exp\big(-\mathtt{i}\int_0^{L+\varepsilon}\lambda^-(y+\xi_{i+1}^-,\tau)dy\big)\big)\exp\big(-\mathtt{i}\int_0^{L}\lambda^-(y+\xi_i^+,\tau)dy\big)}{1-\exp\big(-2\mathtt{i}\int_0^{L+\varepsilon}\lambda^-(y+\xi_{i+1}^-,\tau)dy\big)} \\
&+\frac{\big(\widehat{h}_{i+1}^-(\tau)-\widehat{h}_{i+1}^+(\tau)\exp\big(-\mathtt{i}\int_0^{L+\varepsilon}\lambda^-(y+\xi_{i+1}^-,\tau)dy\big)\big)\exp\big(-\mathtt{i}\int_0^{\varepsilon}\lambda^-(y+\xi_{i+1}^-,\tau)dy\big)}{1-\exp\big(-2\mathtt{i}\int_0^{L+\varepsilon}\lambda^-(y+\xi_{i+1}^-,\tau)dy\big)}.
\end{aligned}$$

Then, one gets

$$\begin{aligned}
\widehat{\mathfrak{e}}_{i}(\tau,\xi_{i+1}^-) &= \frac{\big(\widehat{h}_{i}^+(\tau)-\widehat{h}_{i}^-(\tau)\exp\big(-\mathtt{i}\int_{\xi_{i}^-}^{\xi_{i}^+}\lambda^-(y,\tau)dy\big)\big)\exp\big(\mathtt{i}\int_{\xi_i^+}^{\xi_{i+1}^-}\lambda^-(y,\tau)dy\big)}{1-\exp\big(-2\mathtt{i}\int_{\xi_{i}^-}^{\xi_{i}^+}\lambda^-(y,\tau)dy\big)} \\
&+\frac{\big(\widehat{h}_{i}^-(\tau)-\widehat{h}_{i}^+(\tau)\exp\big(-\mathtt{i}\int_{\xi_{i}^-}^{\xi_{i}^+}\lambda^-(y,\tau)dy\big)\big)\exp\big(-\mathtt{i}\int_{\xi_{i}^-}^{\xi_{i+1}^-}\lambda^-(y,\tau)dy\big)}{1-\exp\big(-2\mathtt{i}\int_{\xi_{i}^-}^{\xi_{i}^+}\lambda^-(y,\tau)dy\big)} \\
&= \frac{\big(\widehat{h}_{i}^+(\tau)-\widehat{h}_{i}^-(\tau)\exp\big(-\mathtt{i}\int_0^{L+\varepsilon}\lambda^-(y+\xi_{i}^-,\tau)dy\big)\big)\exp\big(-\mathtt{i}\int_0^{\varepsilon}\lambda^-(y+\xi_{i+1}^-,\tau)dy\big)}{1-\exp\big(-2\mathtt{i}\int_0^{L+\varepsilon}\lambda^-(y+\xi_{i}^-,\tau)dy\big)} \\
&+\frac{\big(\widehat{h}_{i}^-(\tau)-\widehat{h}_{i}^+(\tau)\exp\big(-\mathtt{i}\int_0^{L+\varepsilon}\lambda^-(y+\xi_{i}^-,\tau)dy\big)\big)\exp\big(-\mathtt{i}\int_0^{L}\lambda^-(y+\xi_{i}^-,\tau)dy\big)}{1-\exp\big(-2\mathtt{i}\int_0^{L+\varepsilon}\lambda^-(y+\xi_{i}^-,\tau)dy\big)}
\end{aligned}$$

Let us set $\widehat{h}_i^{+,(2)}(\tau):=\widehat{\mathfrak{e}}_i(\tau,\xi_{i+1}^-)$ and $\widehat{h}_{i+1}^{-,(2)}(\tau):=\widehat{\mathfrak{e}}_{i+1}(\tau,\xi_i^+)$. Then we are led to

$$\begin{aligned}
\widehat{\mathfrak{e}}_{i+1}^{(2)}(\tau,\xi_i^+) &= \frac{\widehat{\mathfrak{e}}_{i+1}(\tau,\xi_{i+2}^-)-\widehat{\mathfrak{e}}_{i+1}(\tau,\xi_i^+)\exp\big(-\mathtt{i}\int_0^{L+\varepsilon}\lambda^-(y+\xi_{i+1}^-,\tau)dy\big)}{1-\exp\big(-2\mathtt{i}\int_0^{L+\varepsilon}\lambda^-(y+\xi_{i+1}^-,\tau)dy\big)} \\
&\quad\times\exp\big(-\mathtt{i}\int_0^{L}\lambda^-(y+\xi_i^+,\tau)dy\big) \\
&\quad+\frac{\widehat{\mathfrak{e}}_{i+1}(\tau,\xi_i^+)-\widehat{\mathfrak{e}}_{i+1}(\tau,\xi_{i+2}^-)\exp\big(-\mathtt{i}\int_0^{L+\varepsilon}\lambda^-(y+\xi_{i+1}^-,\tau)dy\big)}{1-\exp\big(-2\mathtt{i}\int_0^{L+\varepsilon}\lambda^-(y+\xi_{i+1}^-,\tau)dy\big)} \\
&\quad\times\exp\big(-\mathtt{i}\int_0^{\varepsilon}\lambda^-(y+\xi_{i+1}^-,\tau)dy\big) \\
&= \widehat{h}_{i+1}^-(\tau)\exp\big(-2\mathtt{i}\varepsilon\lambda^-(\tau,\xi_{i+1}^-)\big)+\mathrm{R}_1\big(\tau,\varepsilon,L,\max_{1\leqslant i\leqslant m}\|\widehat{h}_i\|\big)
\end{aligned}$$

and

$$
\begin{aligned}
\widehat{\mathfrak{e}}_i^{(2)}(\tau,\xi_{i+1}^-) &= \frac{\widehat{\mathfrak{e}}_i(\tau,\xi_{i+1}^-)-\widehat{\mathfrak{e}}_i(\tau,\xi_{i-1}^+)\exp\big(-\mathtt{i}\int_0^{L+\varepsilon}\lambda^-(y+\xi_i^-,\tau)dy\big)}{1-\exp\big(-2\mathtt{i}\int_0^{L+\varepsilon}\lambda^-(y+\xi_i^-,\tau)dy\big)} \\
&\quad\times\exp\big(-\mathtt{i}\int_0^{\varepsilon}\lambda^-(y+\xi_{i+1}^-,\tau)dy\big) \\
&\quad+\frac{\widehat{\mathfrak{e}}_i(\tau,\xi_{i-1}^+)-\widehat{\mathfrak{e}}_i(\tau,\xi_{i+1}^-)\exp\big(-\mathtt{i}\int_0^{L+\varepsilon}\lambda^-(y+\xi_i^-,\tau)dy\big)}{1-\exp\big(-2\mathtt{i}\int_0^{L+\varepsilon}\lambda^-(y+\xi_i^-,\tau)dy\big)} \\
&\quad\times\exp\big(-\mathtt{i}\int_0^{L}\lambda^-(y+\xi_i^-,\tau)dy\big) \\
&= \widehat{h}_i^+(\tau)\exp\big(-2\mathtt{i}\varepsilon\lambda^-(\tau,\xi_{i+1}^-)\big)+\mathrm{R}_2\big(\tau,\varepsilon,L,\max_{1\leqslant i\leqslant m}\|\widehat{h}_i\|\big),
\end{aligned}
$$

where $\mathrm{R}_i = O\big(\max_{1\leqslant i\leqslant m}\|\widehat{h}_i\|e^{-\alpha(\tau)L}\big)$. We then have

$$
\widehat{\mathcal{G}}_i^{(C),2}\big(\langle\{\widehat{h}_i^+(\tau),\widehat{h}_{i+1}^-(\tau)\}_i\rangle\big) = C_i(\varepsilon,\tau,V)\langle\big\{\widehat{h}_i^+(\tau),\widehat{h}_{i+1}^-(\tau)\big\}_i\rangle + O\big(\max_{1\leqslant i\leqslant m}\|\widehat{h}_i\|e^{-\alpha(\tau)L}\big).
$$

We yet refer [7], where for large τ, we can rigorously expand the symbol $\lambda^{\pm}$. We do not proceed to this laborious expansions in this paper. In first approximation [7], the local convergence rate between Ω_i,Ω_{i+1} is given by

$$
C_i(\varepsilon,\tau)\approx\exp\big(-\varepsilon\big(\sqrt{2|\tau|}+V(\xi_{i+1}^-)\big)\big).
$$

In general, the above procedure does not allow to directly construct a contraction factor, that is, subdomain-independent coefficients C_i. This is a consequence to the fact that the convergence rate is dependent on the values of the potential at the subdomain interfaces. However we argue that the contraction factor (related to the convergence rate of the CSWR method) $C_\varepsilon^{(C)}$ is such that

$$
\begin{aligned}
\sup_\tau\exp\big(-\varepsilon(\sqrt{2|\tau|}+\max_{i\in\{1,\cdots,m\}}V(\xi_{i+1}^-))\big) \lesssim C_\varepsilon^{(C)} &\lesssim \sup_\tau\exp\big(-\varepsilon(\sqrt{2|\tau|} \\
&\qquad +\min_{i\in\{1,\cdots,m\}}V(\xi_{i+1}^-))\big) \\
&\leqslant \sup_\tau\exp\big(-\varepsilon\sqrt{2|\tau|}\big).
\end{aligned}
$$

The following lemma actually justifies that the convergence rate obtained in the case of m subdomains is close to the one for two subdomains and numerically observed in [7] and in Section 4.

Lemma 2.1. *Let us assume that $f:\boldsymbol{x}\in\mathbb{R}^N\mapsto f(\boldsymbol{x})\in\mathbb{R}^N$, is such that $f(\boldsymbol{x})=\gamma\boldsymbol{x}+\boldsymbol{\varepsilon}$, with $\gamma<1$ and $\|\boldsymbol{\varepsilon}\|=o(\gamma)$. We define the sequence $\boldsymbol{x}_{n+1}=f(\boldsymbol{x}_n)+\varepsilon$, with $\boldsymbol{x}_0\in\mathbb{R}^N$ given. Then, we have*

$$
\|\boldsymbol{x}_{n+1}\|\leqslant\gamma^{n+1}\|\boldsymbol{x}_0\|+o(\gamma).
$$

For $\varepsilon>0$ and $\|V\|_\infty$ small enough, we directly get

$$
C_\varepsilon^{(C)} \approx \sup_\tau\exp\big(-2\mathtt{i}\varepsilon\alpha(\tau)\big).
$$

For the sake of simplicity, we do not detail more the computations. We conclude that, as in the potential-free case the contraction factor for m sufficiently large subdomains ($L \gg 1$) is close to the one for the two-subdomains case.

Proposition 2.3. *The convergence rate $C_\varepsilon^{(C)}$ of the CSWR method with m subdomains of length L is the same as for two-subdomains (see [7]) up to a term of the order of $O\big(e^{-L\sqrt{2|\tau|}}\big)$.*

Although, the convergence rate $C_\varepsilon^{(\mathrm{C})}$ is determined, the overall convergence is also proportional to the number of subdomains due to the $\big(H^{3/4}(t_n, t_{n+1})\big)^{2m}$-norm of $\langle\{h_i^+, h_{i+1}^-\}_{1,\cdots,m}\rangle$. In particular, the transmission from one subdomain to the next one naturally slows down the overall convergence of the SWR method, but without changing the slope of the residual history in logscale (see [7]).

2.3.2. OSWR algorithm

We now consider the OSWR algorithm. More specifically, from time t_n to t_{n+1^-}, the OSWR algorithm with potential reads as follows:

$$\begin{cases} P(\partial_t, \partial_x)\phi_i^{(k)} & = & 0, \qquad (t,x) \in (t_n, t_{n+1}^-) \times \Omega_i, \\ \phi_i^{(k)}(0,\cdot) & = & \varphi_0, \qquad x \in \Omega_i, \\ \big(\partial_x + \mathtt{i}\Lambda^+(\tau,x)\big)\phi_i^{(k)}(t,\xi_i^+) & = & \big(\partial_x + \mathtt{i}\Lambda^+(\tau,x)\big)\phi_{i+1}^{(k-1)}(t,\xi_i^+), \qquad t \in (t_n, t_{n+1}^-), \\ \big(\partial_x + \mathtt{i}\Lambda^-(\tau,x)\big)\phi_i^{(k)}(t,\xi_i^-) & = & \big(\partial_x + \mathtt{i}\Lambda^-(\tau,x)\big)\phi_{i-1}^{(k-1)}(t,\xi_i^-), \qquad t \in (t_n, t_{n+1}^-). \end{cases} \tag{7}$$

The operators $\Lambda^\pm$ are coming from (5) and the corresponding symbols are denoted by $\lambda^\pm$. The latter can be constructed as an asymptotic series of the form (6). In practice, the series $\sum_{j=0}^{+\infty} \lambda_{1/2-j/2}^\pm$ is truncated, and for $p \in \mathbb{N}$, we can define $\lambda_p^\pm := \sum_{j=0}^{p} \lambda_{1/2-j/2}^\pm$ and the corresponding operators $\Lambda_p^\pm$. In [7], the SWR convergence rate is established for the transmission operator $\partial_t \pm \mathtt{i}\Lambda_p^\pm$. In this paper, we will only consider $\Lambda^\pm$. The error equation in Fourier (resp. real) space in time (resp. space) is

$$\begin{cases} \big(\mathtt{i}\tau - V(x) - \partial_x^2\big)\widehat{e}_i(\tau,x) & = & 0, \qquad (\tau,x) \in \mathbb{R} \times \Omega_i, \\ \big(\partial_x + \mathtt{i}\Lambda^\pm(\tau,x)\big)\widehat{e}_i(\tau,\xi^\pm) & = & \widehat{h}_i^\pm(\tau), \qquad \tau \in \mathbb{R}. \end{cases}$$

The analysis of convergence is identical to one presented in Subsubsection 2.2. Basically, we define

$$\mathcal{G}^{(O)} : \langle\big\{h_i^+(t), h_{i+1}^-(t)\big\}_{1\leqslant i\leqslant m}\rangle = \langle\big\{\big(\partial_x + \mathtt{i}\Lambda^+(t,x)\big)e_{i+1}(t,\xi_i^+), \big(\partial_x + \mathtt{i}\Lambda^-(t,x)\big)e_i(t,\xi_{i+1}^-)\big\}_{1\leqslant i\leqslant m}\rangle$$

Thus, we obtain

$$\begin{array}{rcl} \widehat{\mathcal{G}}^{(O)} : \langle\big\{\widehat{h}_i^+(\tau), \widehat{h}_{i+1}(\tau)\big\}_{1\leqslant i\leqslant m}\rangle & = & \langle\big\{\big(\partial_x + \mathtt{i}\lambda^+(\tau,x)\big)\widehat{e}_{i+1}(\tau,\xi_i^+), \\ & & \big(\partial_x + \mathtt{i}\lambda^-(\tau,x)\big)\widehat{e}_i(\tau,\xi_{i+1}^-)\big\}_{1\leqslant i\leqslant m}\rangle. \end{array}$$

We define *approximate* solutions to (7) on each Ω_i, neglecting again the scattering effets

$$\widehat{\mathfrak{e}}_i(\tau,x) \quad = \quad \mathfrak{A}_i(\tau)\exp\big(-\mathtt{i}\int_0^x \lambda^+(y,\tau)dy\big) + \mathfrak{B}_i(\tau)\exp\big(\mathtt{i}\int_0^x \lambda^-(y,\tau)dy\big).$$

Then by construction $\lambda^+ = -\lambda^-$, we get

$$\mathfrak{A}_i(\tau) = \frac{\widehat{h}_i^+(\tau)e^{\int_0^{\xi_i^+}\lambda^+(\tau,y)dy}}{2\mathtt{i}\lambda^+(\tau,x)}, \qquad \mathfrak{B}_i(\tau) = -\frac{\widehat{h}_i^-(\tau)e^{\int_0^{\xi_i^-}\lambda^-(\tau,y)dy}}{2\mathtt{i}\lambda^+(\tau,x)},$$

leading to

$$\begin{array}{rcl}\widehat{\mathcal{G}}^{(O),2} : \langle\big\{\widehat{h}_i^+(\tau), \widehat{h}_{i+1}^-(\tau)\big\}_{1\leqslant i\leqslant m}\rangle & = & \langle\big\{(\partial_x + \mathtt{i}\lambda^+(\tau,x))\widehat{e}_{i+1}^{(2)}(\tau,\xi_i^+), \\ & & (\partial_x - \mathtt{i}\lambda^+(\tau,x))\widehat{e}_i^{(2)}(\tau,\xi_{i+1}^-)\big\}_{1\leqslant i\leqslant m}\rangle \\ & = & \langle\big\{\widehat{h}_{i+2}^+(\tau)e^{-\mathtt{i}\int_{\xi_i^+}^{\xi_{i+2}^+}\lambda^+(\tau,y)}, \widehat{h}_{i-1}^-(\tau)e^{-\mathtt{i}\int_{\xi_{i-1}^-}^{\xi_{i+1}^-}\lambda^+(\tau,y)dy}\big\}_{1\leqslant i\leqslant m}\rangle \\ & = & \langle\big\{\widehat{h}_{i+2}^+(\tau)e^{-2\mathtt{i}\int_0^{L+\varepsilon}\lambda^+(\tau,y+\xi_i^+)}, \widehat{h}_{i-1}^-(\tau)e^{-2\mathtt{i}\int_0^{L+\varepsilon}\lambda^+(\tau,y+\xi_{i-1}^-)dy}\big\}_{1\leqslant i\leqslant m}\rangle .\end{array}$$

We conclude that, as for the CSWR method, the OSWR method has a convergence rate independent, up to a multiplicative constant, of the number of subdomains of length L. Details of the convergence over 2 subdomains for the OSWR and quasi-OSWR can be found in Section 2.3 of [7].

2.4. Scalability

We notice that using a large number of subdomains does not allow for an acceleration of the convergence rate, which is the same as for the 2 subdomain case up to a multiplication coefficient. We however benefit from i) an embarrassingly parallel algorithm, ii) small scale local computations on each subdomain.

3. Extension to time-dependent problems

The principle for analyzing the rate of convergence in the time-dependent equation is roughly speaking identical to the stationary case (see also [8]). Basically, we have to replace t (resp. τ) by $\mathtt{i}t$ (resp. $\mathtt{i}\tau$) in the equations. We denote by $P(\partial_t, \partial_x) = \mathtt{i}\partial_t + \partial_x^2$ the Schrödinger operator, and consider the IBVP on $\Omega = (-a, a)$

$$\left\{\begin{array}{lcll}\big(\mathtt{i}\partial_t + \partial_x^2\big)\phi(t,x) & = & 0, & (t,x) \in (0,T)\times\Omega, \\ \phi(0,\cdot) & = & \varphi_0, & \ \ x \in \Omega, \\ \phi(t,-a) & = & 0, & t \in (0,T), \\ \phi(t,a) & = & 0, & t \in (0,T),\end{array}\right.$$

where $T > 0$ and $\varphi_0 \in L^2(\mathbb{R})$ are given. The convergence rate is defined as the slope of the logarithm residual history according to the Schwarz iteration number, that is $\{(k, \log(\mathcal{E}^{(k)})) : k \in \mathbb{N}\}$, where this time

$$\mathcal{E}^{(k)} := \sum_{i=1}^{m} \Big\| \ \|\phi^{(\mathrm{k})}_{i\big|(\xi_{i+1}^-,\xi_i^+)} - \phi^{(\mathrm{k})}_{i+1\big|(\xi_{i+1}^-,\xi_i^+)}\|_{\infty,\Gamma_\varepsilon}\Big\|_{L^2(0,T)} \leqslant \delta^{\mathrm{Sc}}, \tag{8}$$

δ^{Sc} being a small parameter.

First, the CSWR algorithm reads as follows, for $k \geqslant 1$ and for $i \in \{2, \cdots, m-1\}$:

$$\left\{\begin{array}{lcl} P(\partial_t, \partial_x)\phi_i^{(k)} & = & 0, \qquad (t,x) \in (0,T) \times \Omega_i, \\ \phi_i^{(k)}(0,\cdot) & = & \varphi_0, \qquad x \in \Omega_i, \\ \phi_i^{(k)}(t,\xi_i^+) & = & \phi_{i+1}^{(k-1)}(t,\xi_i^+), \qquad t \in (0,T), \\ \phi_i^{(k)}(t,\xi_i^-) & = & \phi_{i-1}^{(k-1)}(t,\xi_i^-), \qquad t \in (0,T). \end{array}\right.$$

In Ω_1, we get

$$\left\{\begin{array}{lcl} P(\partial_t, \partial_x)\phi_1^{(k)} & = & 0, \qquad (t,x) \in (0,T) \times \Omega_1, \\ \phi_1^{(k)}(0,\cdot) & = & \varphi_0, \qquad x \in \Omega_1, \\ \phi_1^{(k)}(t,-a) & = & 0, \qquad t \in (0,T), \\ \phi_1^{(k)}(t,\xi_1^+) & = & \phi_2^{(k-1)}(t,\xi_2^+), \qquad t \in (0,T), \end{array}\right.$$

and in Ω_m

$$\left\{\begin{array}{lcl} P(\partial_t, \partial_x)\phi_m^{(k)} & = & 0, \qquad (t,x) \in (0,T) \times \Omega_m, \\ \phi_m^{(k)}(0,\cdot) & = & \varphi_0, \qquad x \in \Omega_m, \\ \phi_i^{(k)}(t,\xi_m^-) & = & \phi_{m-1}^{(k-1)}(t,\xi_m^-), \qquad t \in (0,T), \\ \phi_m^{(k)}(t,+a) & = & 0, \qquad t \in (0,T). \end{array}\right.$$

In order to analyze the convergence of the SWR methods, it is sufficient to repace τ by $-\mathtt{i}\tau$ in all the equations from Section 2. In particular, for m subdomains, we can write that

$$\widehat{\mathcal{G}}^{(C),2}\big(\langle\{\widehat{h}_i^+(\tau), \widehat{h}_{i+1}^-(\tau)\}_i\rangle\big) \quad = \quad e^{-2\beta(\tau)\varepsilon}\big\langle\big\{\widehat{h}_i^+(\tau), \widehat{h}_{i+1}^-(\tau)\big\}_i\big\rangle + O\big(e^{-\alpha(\tau)L}\big),$$

where $\beta(\tau) := \sqrt{\tau}$.

A similar study is possible with OSWR algorithm for m subdomains. First, define the transparent operator $\partial_x \pm e^{-\mathtt{i}\pi/4}\partial_t^{1/2}$ at the interfaces. The OSWR algorithm reads as follows: for $k \geqslant 1$ and for $i \in \{2, \cdots, m-1\}$

$$\left\{\begin{array}{lcl} P(\partial_t, \partial_x)\phi_i^{(k)} & = & 0, \qquad (t,x) \in (t_n,t_{n+1}^-) \times \Omega_i, \\ \phi_i^{(k)}(0,\cdot) & = & \varphi_0, \qquad x \in \Omega_i, \\ (\partial_x + e^{-\mathtt{i}\pi/4}\partial_t^{1/2})\phi_i^{(k)}(t,\xi_i^+) & = & (\partial_x + e^{-\mathtt{i}\pi/4}\partial_t^{1/2})\phi_{i+1}^{(k-1)}(t,\xi_i^+), \qquad t \in (t_n,t_{n+1}^-), \\ (\partial_x - e^{-\mathtt{i}\pi/4}\partial_t^{1/2})\phi_i^{(k)}(t,\xi_i^-) & = & (\partial_x - e^{-\mathtt{i}\pi/4}\partial_t^{1/2})\phi_{i-1}^{(k-1)}(t,\xi_i^-), \qquad t \in (t_n,t_{n+1}^-). \end{array}\right.$$

In Ω_1, we get

$$\left\{\begin{array}{lcl} P(\partial_t, \partial_x)\phi_1^{(k)} & = & 0, \qquad (t,x) \in (t_n,t_{n+1}^-) \times \Omega_1, \\ \phi_1^{(k)}(0,\cdot) & = & \varphi_0, \qquad x \in \Omega_1, \\ \phi_1^{(k)}(t,-a) & = & 0, \qquad t \in (t_n,t_{n+1}^-), \\ (\partial_x + e^{-\mathtt{i}\pi/4}\partial_t^{1/2})\phi_1^{(k)}(t,\xi_1^+) & = & (\partial_x + e^{-\mathtt{i}\pi/4}\partial_t^{1/2})\phi_2^{(k-1)}(t,\xi_1^+), \qquad t \in (t_n,t_{n+1}^-), \end{array}\right.$$

and in Ω_m

$$\begin{cases} P(\partial_t, \partial_x)\phi_m^{(k)} & = & 0, \qquad (t,x) \in (t_n, t_{n+1}^-) \times \Omega_m, \\ \phi_m^{(k)}(0,\cdot) & = & \varphi_0, \qquad x \in \Omega_m, \\ (\partial_x - e^{-\mathtt{i}\pi/4}\partial_t^{1/2})\phi_i^{(k)}(t,\xi_m^-) & = & (\partial_x - e^{-\mathtt{i}\pi/4}\partial_t^{1/2})\phi_{m-1}^{(k-1)}(t,\xi_m^-), \qquad t \in (t_n, t_{n+1}^-), \\ \phi_m^{(k)}(t,+a) & = & 0, \qquad t \in (t_n, t_{n+1}^-). \end{cases}$$

We then consider

$$\begin{cases} \big(\mathtt{i}\tau - \partial_x^2\big)\widehat{e}_i(\tau,x) & = & 0, \qquad (\tau,x) \in \mathbb{R} \times \Omega_i, \\ (\partial_x \pm \beta(\tau))\widehat{e}_i(\tau,\xi^{\pm}) & = & \widehat{h}_i^{\pm}(\tau), \qquad \tau \in \mathbb{R}, \end{cases}$$

where we have set $\beta(\tau) := e^{\mathtt{i}\pi/4}\sqrt{\tau}$, and we get: $\widehat{e}_i(\tau,x) = A_i(\tau)e^{\beta(\tau)x} + B_i(\tau)e^{-\beta(\tau)x}$. From the boundary conditions, we find, for $i \in \{2, \cdots, m-1\}$,

$$A_i(\tau) = \frac{\widehat{h}_i^+(\tau)e^{-\beta(\tau)\xi_i^+}}{2\beta(\tau)}, \qquad B_i(\tau) = -\frac{\widehat{h}_i^-(\tau)e^{\beta(\tau)\xi_i^-}}{2\beta(\tau)}.$$

We introduce a mapping $\mathcal{G}^{(O)}$ defined as follows

$$\begin{aligned} &\mathcal{G}^{(O)} : \langle \big\{h_i^+(t), h_{i+1}^-(t)\big\}_{1\leqslant i\leqslant m}\rangle \\ &\quad = \langle \big\{(\partial_x + e^{-\mathtt{i}\pi/4}\partial_t^{1/2})e_{i+1}(t,\xi_i^+), (\partial_x - e^{-\mathtt{i}\pi/4}\partial_t^{1/2})e_i(t,\xi_{i+1}^-)\big\}_{1\leqslant i\leqslant m}\rangle. \end{aligned}$$

We again find the same convergence rate as in [8] for 2 subdomain, but the overall error is still shifted in logscale, by a positive constant linearly dependent on $\log(m)$.

4. Numerical experiments

4.1. Eigenvalue problem

We present a simple test case illustrating the theoretical results presented in Section 2. We take $V(x) = 5x^2/2$, and $\Omega = (-2,2)$ and we solve the Schrödinger equation in imaginary-time using a three-points finite difference scheme, with meshsize $\Delta x = 1/64$, and for a time step $\Delta t = 0.2$. Details about the solver can be found in [7]. We apply the CSWR method on $m = 2, 4, 8$ subdomains and compare the convergence rate as a function of the Schwarz iterations. Initially, we take $\phi_0(x) = \widetilde{\phi}_0(x)/\|\widetilde{\phi}_0\|_2$, with $\phi_0(x) = e^{-4x^2}$. The $m-1$ overlapping zones have a length equal to $\varepsilon = \Delta x$, corresponding to 2 nodes. We observe that the asymptotic residual history is numerically independent of the number of subdomains, see Fig. 2.

We also report on Fig. 3 the converged solution $\big\{(x, \phi^{\mathrm{cvg},(k^{(\mathrm{cvg})})}(x) = \phi_g(x)),\, x \in (-2,2)\big\}$, the initial guess $\big\{(x, \phi_0(x)),\, x \in (-2,2)\big\}$, as well as the NGF converged solution after 20 Schwarz iterations with 8 subdomains, $\{(x, \phi^{\mathrm{cvg},(20)}(x)),\, x \in (-2,2)\}$. We however numerically observe that for 8 subdomains the asymptotic rates of convergence seems to be relatively different than 2 and 4. This can be explained by the fact that for a large number of subdomains, the size of each of these subdomains is relatively small, which induces an inaccuracy in the theoretical slope of convergence. In addition, the overall convergence rate depends on the value of the potential at the subdomain interfaces. In the next example, the overall domain is larger, leading to larger subdomain, then better accuracy of the convergence rate.

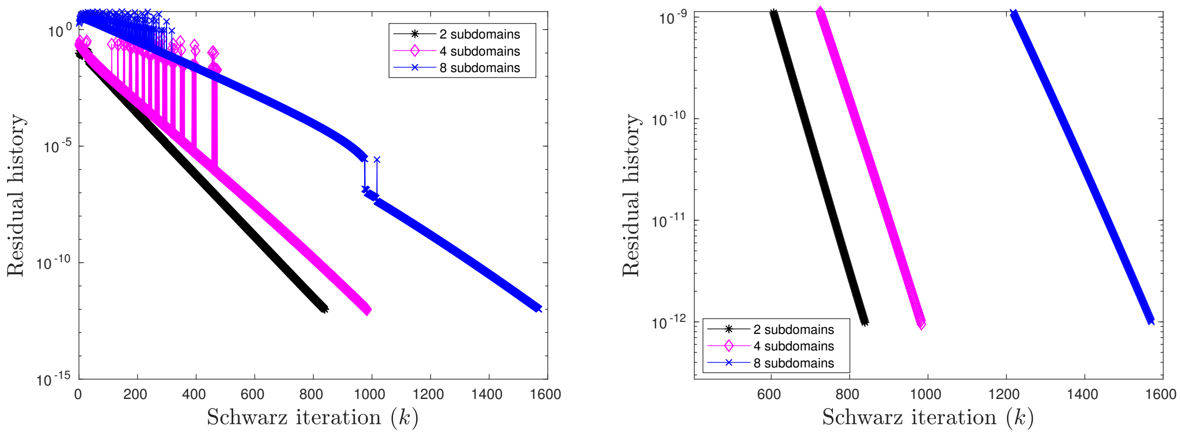

Figure 2: Comparison of the asymptotic convergence rates for 2, 4 and 8 subdomains, including a zoom in the asymptotic regime.

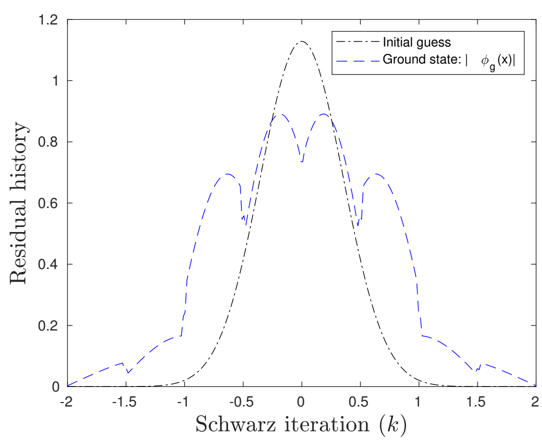

Figure 3: Initial guess, potential and converged ground state.

4.2. Time-dependent equation

In this example the potential is chosen as $V(x) = -5\exp(-2x^2)$, with $\Omega = (-8, 8)$ and final time $T = 10$. We solve the Schrödinger equation in real-time with the three-points finite difference scheme, for $\Delta x = 1/32$ and $\Delta t = 10^{-2}$. We refer to [8] for the details concerning the solver. The CSWR method is applied for $m = 2$, 4, 8 and 16 subdomains. We compare the convergence rate as a function of the Schwarz iterations. Initially, we take $\phi_0(x) = \widetilde{\phi}_0(x)/\|\widetilde{\phi}_0\|_2$, with $\phi_0(x) = \pi^{-1/4}e^{-5(x+2)^2+\mathrm{i}k_0x}$, for $k_0 = 5$. The $m-1$ overlapping zones have a length equal to $\varepsilon = \Delta x$, corresponding to 2 nodes. We observe on Fig. 4 that, as proven above, the asymptotic residual history is independent of the number of subdomains.

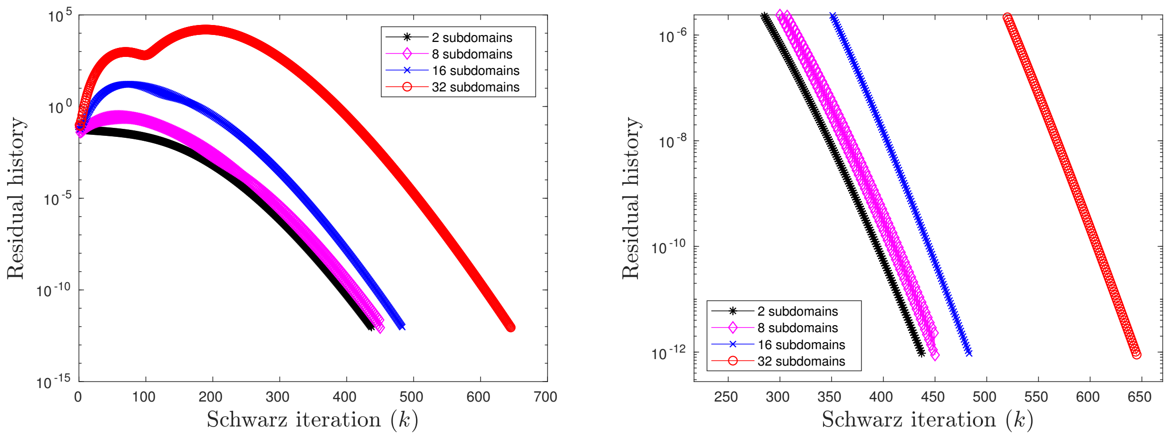

Figure 4: Comparison of the asymptotic convergence rates for 2,, 8, 16 and 32 subdomains, including a zoom in the asymptotic regime.

We also report in Fig. 5 the amplitude of the converged solution $\big\{(x, |\phi^{N,(k^{(\mathrm{cvg})})}(x)|, x \in (-8, 8)\big\}$, the initial guess $\big\{(x, |\phi_0(x)|), x \in (-8, 8)\big\}$, as well as the TDSE converged solution after 10 Schwarz iterations with 16 subdomains, $\big\{(x, |\phi^{N,(7)}(x)|), x \in (-8, 8)\big\}$, where N is such that $T_N = T = 10$.

5. Conclusion

In this paper, we presented an asymptotic analysis of the convergence rate of the multi-domains CSWR and OSWR methods for the 1D linear Schrödinger equation in imaginary- and real-time. Asymptotic estimates show that the already existing estimates stated for the two-domains configuration extend here to m domains. This is illustrated through some numerical examples.

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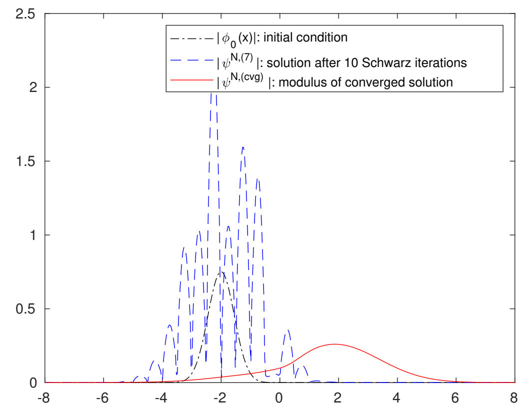

Figure 5: Amplitudes of the initial guess, converged solution and solution after 7 Schwarz iterations on 16 subdomains.

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